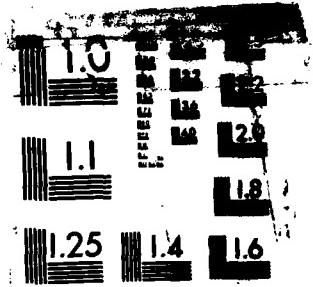


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July 4, 1986

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Contract DAJA45-86-C-0004
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First Interim Report: April 18, 1986

QUANTUM TRANSPORT AND MONTE CARLO TECHNIQUES

Since the end of the previous contract (DAJA45-83-C-0039), a major improvement toward a Monte Carlo solution of the Liouville quantum transport equation for the density matrix $\hat{\rho}^{(e)}(E, E')$ of an ensemble of electrons in a crystal interacting with phonons and with an external electric field has been accomplished. It consisted in moving from a finite-difference formulation of the time-evolution equation of the density matrix to an iterative expansion of its integral form:

$$\begin{aligned}\hat{\rho}^{(e)}(E, E', t) &= \hat{\rho}^{(e)}(E, E', 0) + \hat{\rho}^{(e)(1)}(E, E', t) + \hat{\rho}^{(e)(2)}(E, E', t) + \dots \\ &= \hat{\rho}^{(e)}(E, E', 0) + \sum_{\langle n_q \rangle} \int_0^t dt_1 \left[[H_{ep}(t_1), \hat{\rho}^{(e)(0)}] \right] (E, \{n_q\}, E', \{n_q\}) + \\ &\quad + \int_0^t dt_1 \int_0^{t_1} dt_2 \left[[H_{ep}(t_2), [H_{ep}(t_1), \hat{\rho}^{(e)(0)}]] \right] (E, \{n_q\}, E', \{n_q\}) + \dots\end{aligned}$$

where H_{ep} is the electron-phonon interaction hamiltonian, \vec{k} and $\langle n_q \rangle$ are the electron and phonon coordinates, respectively.

From the analytical development of the various perturbative corrections $\hat{\rho}^{(e)(n)}(t)$, it is found that:

- (i) the zero-order term is the ballistic translation during the interval $(0, t)$ due to the action of the external

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electric field;

(ii) if we want to evaluate mean values of electron operators $\hat{A}(k)$ that are diagonal on the set of states $|k\rangle$ used to define the density matrix, only the diagonal terms of $\hat{\rho}^{(e)}$ are involved in the trace operation:

$$\langle \hat{A} \rangle = \text{Trace} (\hat{\rho} \hat{A}) \quad (2)$$

It can be proved analytically that every odd perturbative correction $\hat{\rho}_{kk}^{(even)}(E, E', t)$ is zero if the initial condition for the total density matrix of the electron and phonon system is decoupled into a product of the electron and the phonon part.

(iii) all the even perturbative corrections $\hat{\rho}_{kk}^{(even)}(t)$ can be written as sums of terms, and each term can be described as a product of real and virtual phonon absorptions and emissions.

The numerical procedure for the solution of Eq.(1) is being developed.

An oral communication about this recent work (abstract here enclosed) has been submitted and accepted at the next International Conference of Semiconductors. It will be presented in Stockholm this coming august.

A preliminary paper on this subject has been presented and discussed at the recent Workshop on the Physics of Ultrasmall and Quantum Structured Devices (Tempe, December 1985). The preprint is also enclosed (C. Jacoboni et al., to be published in Superlattice and Microstructures).

→ HOT-PHONONS IN SEMICONDUCTORS, *Kinetic theory of hot phonons in semiconductors*

We have recently started a project to study non-equilibrium phonon effects in semiconductors using Monte Carlo techniques. It is well known that under the application of a sufficiently strong electric field, the mean energy of the carriers exceed the thermal one. Within this "hot electron" regime, the phonon distribution can be also shifted from its thermal equilibrium. This, in turn, can significantly influence the low-temperature transport in semiconductors.

The research is done in collaboration with Prof. Kocevar of the Physics Department of the University of Graz, Austria. The initial stage of this collaboration has focused



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on the development of a novel Monte Carlo procedure that includes phonon disturbances in the analysis of steady-state high field transport in p-Ge at low temperatures. The algorithm is based on the iterative solution of the coupled Boltzmann equations for carriers and phonons. At each iterative step the phonon distribution is taken from an analytical model parameterized by the carrier mean energy and drift velocity, and is feeded into the Monte Carlo simulation at the following iteration.

The first results have been presented at the 4th International Conference on Hot Electrons in Semiconductors, Innsbruck 1985 (see P. Bordone et al., Physica 134b, 169 *includ* (1985)). At the lowest electric fields, the phonon perturbation produces an increase of the drift velocity (drag effect), while at the higher fields the frictional effect of the enhanced phonon population dominates, leading to a decrease in the drift velocity. A more extensive discussion will be submitted for publication shortly.

A full Monte Carlo technique for both carriers and phonons is now under development for the case of the relaxation of photo-excited electrons in bulk GaAs and in GaAs-AlGaAs quantum wells. A copy of the abstract submitted and accepted at the next International Conference on the Physics of Semiconductors (Stockholm, Aug. 1986) is also included.

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